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L1 31 (REDUCED (3A) DIMENS?) (S) ("NULCEAR MAGNETIC" OR NMR)
L2 34 (REDUCED (3A) DIMENS?) (S) ("NUCLEAR MAGNETIC" OR NMR)

L2 ANSWER 1 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:485059 CAPLUS
DOCUMENT NUMBER: 137:105922
TITLE: "Reduced-dimensionality NMR spectroscopy for high-throughput protein resonance assignment"
AUTHOR(S): *Szyperski, Thomas; Yeh, Deok C.; Sukumaran, Dinesh K.; Moseley, Hunter N. B.; Montelione, Gaetano T.*
CORPORATE SOURCE: Departments of Chemistry and Structural Biology, State University of New York, Buffalo, NY, 14260, USA
SOURCE: **Proceedings of the National Academy of Sciences of the United States of America (2002), 99(12), 8009-8014**
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A suite of reduced-dimensionality 13C,15N,1H-triple- resonance NMR expts. is presented for rapid and complete protein resonance assignment. Even when using short measurement times, these expts. allow one to retain the high spectral resolution required for efficient automated anal. "Sampling limited" and "sensitivity limited" data collection regimes are defined, resp., depending on whether the sampling of the indirect dimensions or the sensitivity of a multidimensional NMR expts. per se dets. the minimally required measurement time. We show that reduced-dimensionality NMR spectroscopy is a powerful approach to avoid the "sampling limited regime"-i.e., a standard set of ten expts. proposed here allows one to effectively adapt minimal measurement times to sensitivity requirements. This is of particular interest in view of the greatly increased sensitivity of NMR spectrometers equipped with cryogenic probes. As a step toward fully automated anal., the program AUTOASSIGN has been extended to provide sequential backbone and 13C<SYM98> resonance assignments from these reduced-dimensionality NMR data. REFERENCE COUNT: 28

L2 ANSWER 2 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:322738 CAPLUS
DOCUMENT NUMBER: 137:29617
TITLE: "Letter to the editor: 1H, 13C, and 15N resonance assignments and secondary structure of the PWI domain from SRm160 using reduced dimensionality NMR"
AUTHOR(S): *Szymczyna, Blair R.; Pineda-Lucena, Antonio; Mills, Jeffrey L.; Szyperski, Thomas; Arrowsmith, Cheryl H.*
CORPORATE SOURCE: Division of Molecular and Structural Biology, Ontario Cancer Institute and Department of Medical Biophysics, University of Toronto, Toronto, ON, M5G 2M9, Can.

SOURCE: **Journal of Biomolecular NMR (2002), 22(3), 299-300**
CODEN: JBNME9; ISSN: 0925-2738
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The nearly complete 1H, 13C, and 15N resonance assignments and secondary structure of a 12.5 kDa polypeptide containing the PWI motif of the SR-related nuclear matrix associated protein of 160 kDa (SRm160) are reported. The PWI motif is highly conserved in homologs of SRm160 and other splicing or splicing-related proteins. The assignments will serve as the basis for computing the domain's three-dimensional solution structure, which will help elucidate its possible role in pre-mRNA processing. A fragment of human SRm160 encoding amino acids 27-134, which includes the PWI motif, was cloned into the pET-15b expression vector and expressed in Escherichia coli BL21-Gold cells. Reduced dimensionality NMR expts. facilitated resonance assignment by resolving chemical shift degeneracies and providing addnl. correlations not observed in conventional 3D NMR expts. The assignments of the PWI motif are virtually complete. The backbone is completely assigned and every backbone amide resonance is accounted for in the [15N, 1H]-HSQC, with the exception of residual histidine tag amino acids at the N-terminus. REFERENCE COUNT: 9

L2 ANSWER 8 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1998:470026 CAPLUS
DOCUMENT NUMBER: 129:199994
TITLE: "Sequential resonance assignment of medium-sized 15N/13C-labeled proteins with projected 4D triple resonance NMR experiments"
AUTHOR(S): *Szyperski, Thomas; Banecki, Bogdan; Braun, Daniel; Glaser, Ralf W.*
CORPORATE SOURCE: Institut fur Molekularbiologie und Biophysik, Eidgenossische Technische Hochschule-Honggerberg, Zurich, CH-8093, Switz.
SOURCE: **Journal of Biomolecular NMR (1998), 11(4), 387-405**
CODEN: JBNME9; ISSN: 0925-2738
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We recently introduced a new line of reduced- dimensionality expts. making constructive use of axial peak magnetization, which has so far been suppressed as an undesirable artifact in multidimensional NMR spectra. The peaks arising from the axial magnetization are located at the center of the doublets resulting from projection. Here we describe the use of such projected four-dimensional (4D) triple resonance expts. for the efficient sequential resonance assignment of 15N/13C-labeled proteins. A 3D H<SYM97>/<SYM98> C<SYM97>/<SYM98>(CO)NHN experiment is recorded either in conjunction with 3D HNN<CO,CA> or with the newly presented 3D HNNCAHA scheme. The first combination yields sequential assignments based on the measurement of 13C<SYM97> chemical shifts and provides a complete 1H, 13C and 15N resonance assignment of polypeptide backbone and CHn<SYM98> moieties. When employing the second combination, 13C:O chemical shifts are not measured, but the sequential assignment relies on both 13C<SYM97> and 1H<SYM97> chemical shifts. The

assignment is performed in a semi-automatic fashion using the program XEASY in conjunction with the newly implemented program SPSCAN. This program package offers routines for the facile mutual interconversion of single-quantum and zero/double-quantum frequencies detected in conventional and reduced-dimensionality spectra, resp. In particular, SPSCAN comprises a peak picking routine tailored to cope with the distinct peak patterns of projected NMR expts. performed with simultaneous acquisition of central peaks. Data were acquired at 13° for the N-terminal 63-residue polypeptide fragment of the 434 repressor. Anal. of these spectra, which are representative for proteins of about 15 kDa when working at commonly used temps. around 30°, demonstrates the efficiency of our approach for the assignment of medium-sized 15N/13C doubly labeled proteins. REFERENCE COUNT: 91

L2 ANSWER 12 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:479407 CAPLUS
DOCUMENT NUMBER: 125:130549
TITLE: "Useful Information from Axial Peak Magnetization in Projected NMR Experiments"
AUTHOR(S): *Szyperski, T.; Braun, D.; Banecki, B.; Wuethrich, K.*
CORPORATE SOURCE: Institut fuer Molekularbiologie und Biophysik, Eidgenoessische Technische Hochschule-Hoenggerberg, Zurich, CH-8093, Switz.
SOURCE: **Journal of the American Chemical Society (1996), 118(34), 8146-8147**
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Axial peaks in multidimensional NMR expts. are usually suppressed by phase cycling or the application of pulsed field gradients. This communication shows that in reduced-dimensionality NMR spectra axial peak magnetization can provide valuable addnl. information, as peaks which are located at the center of the doublets arising from the projection. These central peaks facilitate both the unambiguous assignment of multiple doublets with degenerate chemical shifts in the other dimensions, and the symmetrization of the spectrum. Using presently proposed techniques, simultaneous acquisition of projected and central peaks in reduced-dimensionality NMR spectroscopy can be achieved without addnl. expense of instrument time.

L2 ANSWER 14 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:27748 CAPLUS
DOCUMENT NUMBER: 125:87206
TITLE: "A Novel Reduced-Dimensionality Triple-Resonance Experiment for Efficient Polypeptide Backbone Assignment, 3D CO HN N CA". [Erratum to document cited in CA123:340904]
AUTHOR(S): Szyperski, Thomas; Braun, Daniel; Fernandez, Cesar; Bartels, Christian; Wuthrich, Kurt
CORPORATE SOURCE: Switz.
SOURCE: Journal of Magnetic Resonance, Series B (1995), 109(3), 339
CODEN: JMRBE5; ISSN: 1064-1866

PUBLISHER: Academic
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The errors were not reflected in the abstract or the index entries.

L2 ANSWER 18 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:97105 CAPLUS
DOCUMENT NUMBER: 122:213455
TITLE: New approaches to computer-aided NMR interpretation and structure prediction
AUTHOR(S): Maier, Walter
CORPORATE SOURCE: BASF AG, Ludwigshafen, Germany
SOURCE: Comput.-Enhanced Anal. Spectrosc. (1993), Volume 4, 37-55. Editor(s): Wilkins, Charles L. Plenum: New York, N. Y.
CODEN: 56VWA6
DOCUMENT TYPE: Conference
LANGUAGE: English
AB SpecEdit is a PC-based interface software between NMR spectrometers and the SpecInfo database system. SpecEdit allows the archiving of reduced 1H and 13C NMR data. It can be used as a tool for routine automatic interpretation of reduced 1-dimension NMR spectra of typical organic mols., library searching, and structure prediction. SpecEdit offers a graphic mouse, and a keyboard-driven editor for the expert. Powerful functions for interpretation, spectral editing, and easy handling of SpecInfo structures are available. Structure assignment of peaks can be done within seconds with mouse clicks.

L2 ANSWER 20 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1994:207119 CAPLUS
DOCUMENT NUMBER: 120:207119
TITLE: Reduced dimensionality in triple-resonance NMR experiments. [Erratum to document cited in CA119(18):194184g]
AUTHOR(S): Szyperski, T.; Wider, G.; Bushweller, J. H.; Wuethrich, K.
CORPORATE SOURCE: Inst. Molekularbiol. Biophys., Eidg. Tech. Hochsch.-Hoenggerberg, Zurich, CH-8093, Switz.
SOURCE: Journal of the American Chemical Society (1994),116(4), 1601
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The errors were not reflected in the abstract or the index entries.

L2 ANSWER 21 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1993:594184 CAPLUS
DOCUMENT NUMBER: 119:194184
TITLE: "Reduced dimensionality in triple-resonance NMR experiments"
AUTHOR(S): Szyperski, T.; Wider, G.; Bushweller, J. H.; Wuethrich, K.
CORPORATE SOURCE: Inst. Molekularbiol. Biophys., Eidg. Tech. Hochsch.-Hoenggerberg, Zurich, CH-8093, Switz.
SOURCE: Journal of the American Chemical Society (1993), 115(20), 9307-8

CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new projection technique is presented for reducing the dimensionality of triple-resonance NMR expts. that delineate exclusively scalar connectivities. The technique makes use of the fact that any two nuclei that can be independently excited may be observed in a common dimension by simultaneous incrementation of their chemical shift evolution periods. All triple-resonance pulse sequences that were implemented so far are amenable to such a reduction in dimensionality. Advantages are that without loss of the potentialities of the higher-dimensional expts., longer maximal evolution times can be chosen in the indirect dimensions, more extensive phase cycling is feasible within the same accumulation time, and the reduced data size facilitates the data handling and processing. Practical applications include the replacement of 4-dimensional triple-resonance schemes by 3-dimensional expts., and the use of 2-dimensional triple-resonance expts. for studies of smaller mols., for example, receptor-bound isotope-labeled polypeptide ligands.

L2 ANSWER 25 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1991:472224 CAPLUS
DOCUMENT NUMBER: 115:72224
TITLE: Assignment of protein NMR spectra in the light of homonuclear 3D spectroscopy: an automatable procedure based on 3D TOCSY-TOCSY and 3D TOCSY-NOESY
AUTHOR(S): Oschkinat, H.; Holak, T. A.; Cieslar, C.
CORPORATE SOURCE: Max-Planck Inst. Biochem., Martinsried, D-8033, Germany
SOURCE: Biopolymers (1991), 31(6), 699-712
CODEN: BIPMAA; ISSN: 0006-3525
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Automated assignment of proteins is greatly simplified using data from 3-dimensional NMR spectra. A strategy is presented which makes use of 3D-TOCSY-TOCSY and 3D-TOCSY-NOESY; its potential is demonstrated with the example of the spectra of bovine pancreatic trypsin inhibitor. The discussion of the potential of 3-dimensional NMR includes the introduction of a simple graph for the description of the information content of multidimensional NMR spectra.

L2 ANSWER 34 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1981:628727 CAPLUS
DOCUMENT NUMBER: 95:228727
TITLE: The accordion experiment, a simple approach to three-dimensional NMR spectroscopy
AUTHOR(S): Bodenhausen, Geoffrey; Ernst, R. R.
CORPORATE SOURCE: Lab. Phys. Chem., Eidg. Tech. Hochsch., Zurich, 8092, Switz.
SOURCE: Journal of Magnetic Resonance (1969-1992) (1981), 45(2), 367-73
CODEN: JOMRA4; ISSN: 0022-2364

DOCUMENT TYPE: Journal
LANGUAGE: English
AB As a simple approach to 3-dimensional NMR spectroscopy a novel type of experiment is proposed in which the dimension is reduced from 3 to 2 by synchronous incrementation of evolution period t, and the mixing time tm parameters: tm = Kt1. Because of the concerted stretching of the pulse sequence, this experiment is referred to as accordion spectroscopy. The salient feature of the novel experiment is the accommodation of 2-dimensional information along a single time or frequency axis. In complete analogy to standard 2-dimensional exchange spectroscopy, the peak positions in an accordion spectrum characterize the origin (<SYM119>1) and destination (<SYM119>2) of the exchanging magnetization. The 3rd dimension (<SYM119>m) is reflected in the lineshape along the <SYM119>1, <SYM119>m axis. These lineshapes correspond to Fourier transforms with respect to tm of the mixing functions aii(tm) and aij(tm), and contain all information relevant to the dynamic processes. These mixing functions can be retrieved from an accordion spectrum by a 3rd (reverse) Fourier transformation for any pair of sites i and j.